Bindung in mehratomigen Molekülen: Hybridorbitale

„Berylliumhydrid BeH_2“

BeH_2 ist als Monomer nicht existent. Es dient hier als Modellverbindung für das lineare $Be(CH_3)_2$.

$H_3C—Be—CH_3$ " H—Be—H "

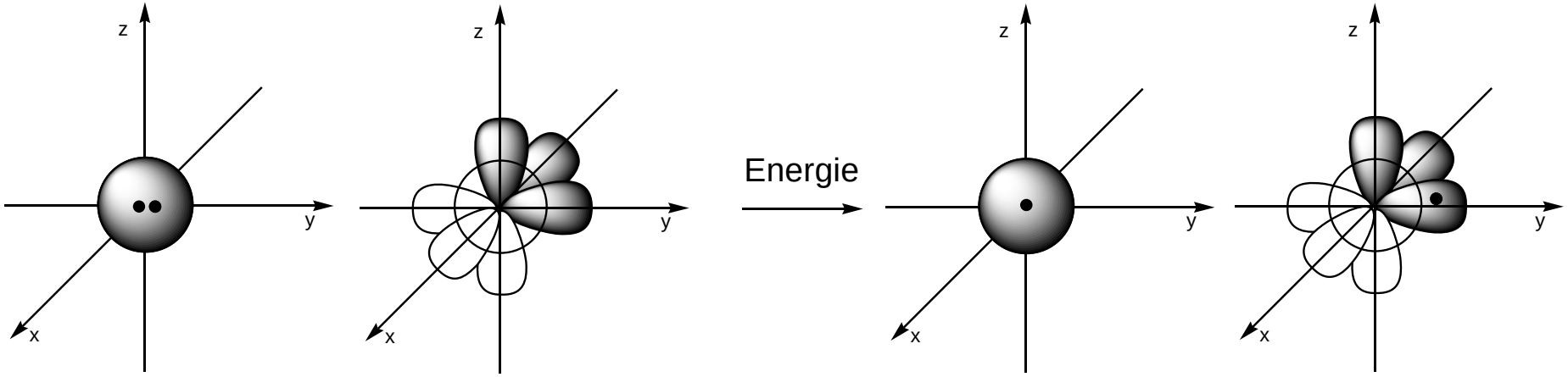
Elektronenkonfiguration: Be ($1s^2$, $2s^2$)

Be (Grundzustand)

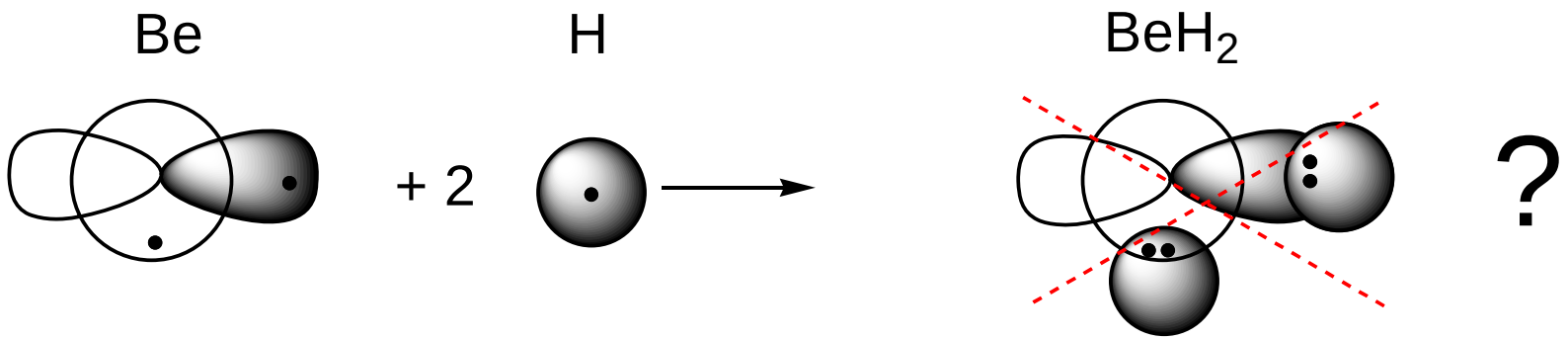
Be: $2s^2\ 2p_x^0\ 2p_y^0\ 2p_z^0$

Be* (angeregter Zustand)

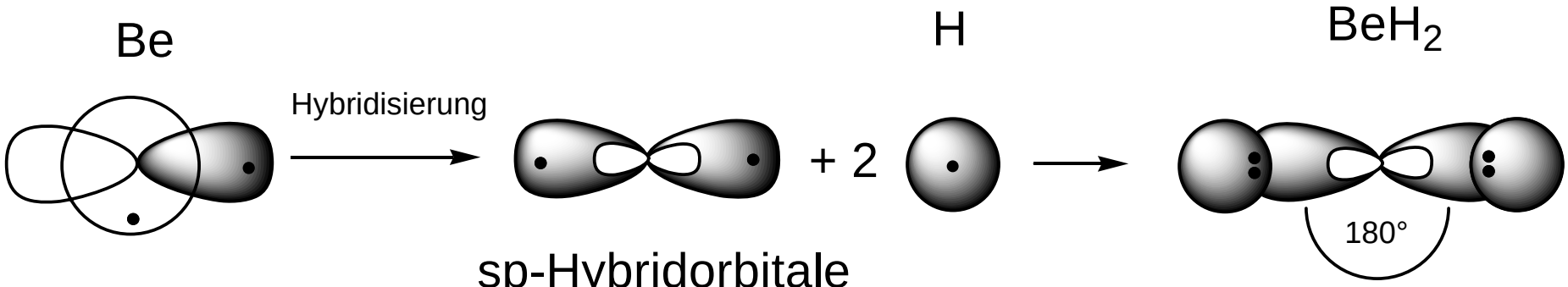
Be*: $2s^1\ 2p_x^1\ 2p_y^0\ 2p_z^0$



s-AO p_x-, p_y-, p_z-AO s-AO p_x-, p_y-, p_z-AO



Dieses BeH_2-Molekül hätte unterschiedliche Bindungslängen und wäre gewinkelt.

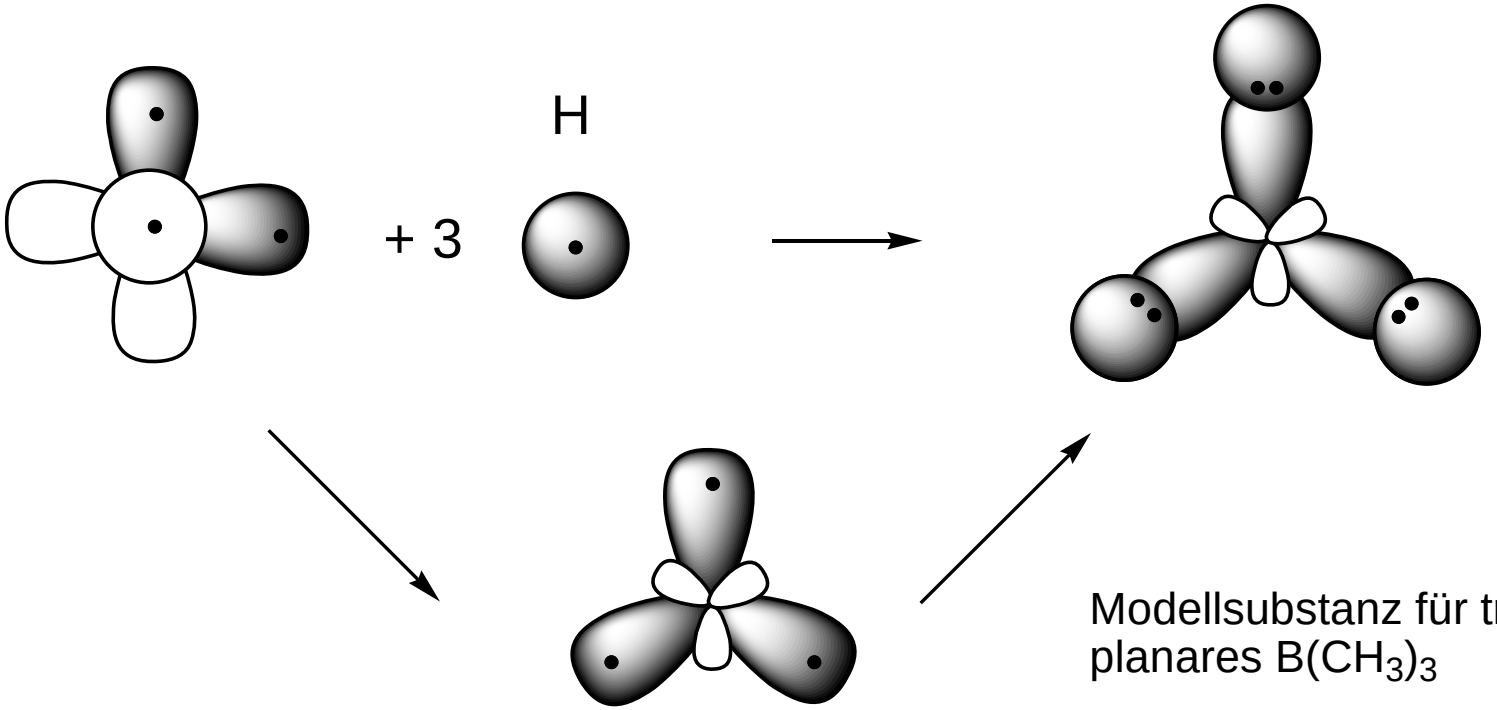


sp-Hybridorbitale

B* (angeregter Zustand)

B*: $2s^1\ 2p_x^1\ 2p_y^1\ 2p_z^0$

" BH_3 "



drei sp^2-Hybridorbitale

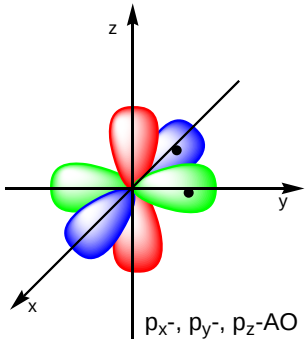
Bindungswinkel: 120°

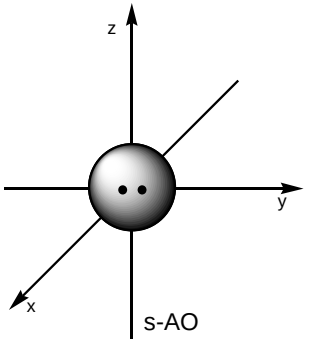
Modellsubstanz für trigonal-planares $B(CH_3)_3$

Bindungsverhältnisse im Methan CH_4

C (Grundzustand)

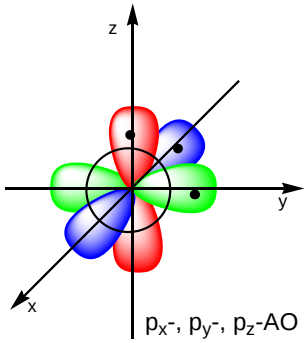
C: $2s^2$ $2p_x^1$ $2p_y^1$ $2p_z^0$

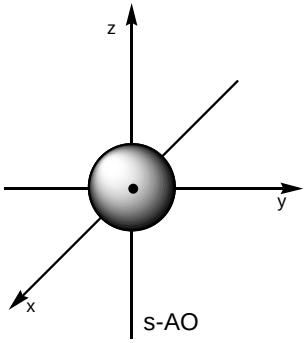




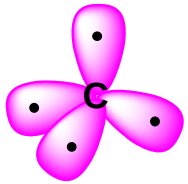
C* (angeregter Zustand)

C*: $2s^1$ $2p_x^1$ $2p_y^1$ $2p_z^1$



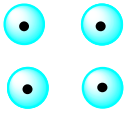


C* (hybridisierter Zustand = "Valenzzustand")

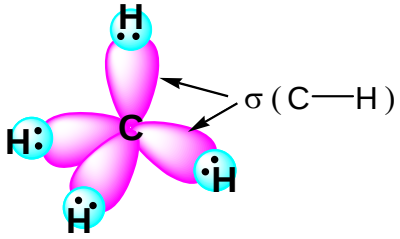


sp^3-Hybrid-AO

+ 4 H· H: $1s^1$



CH_4-Tetraeder

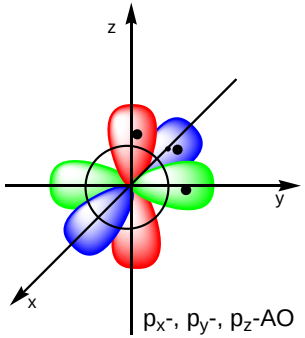


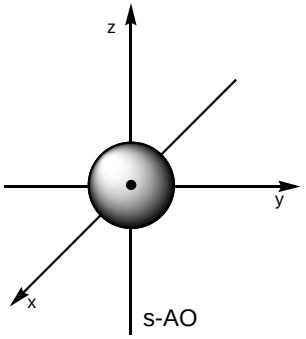
Bindungswinkel HCH: 109.5°

Bindungsverhältnisse im Ethen C_2H_4

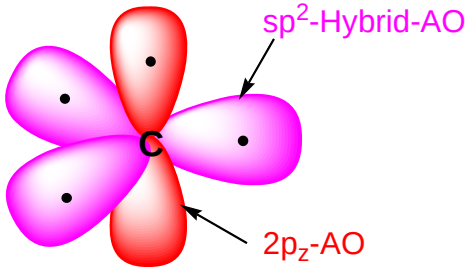
C* (angeregter Zustand)

C*: $2s^1$ $2p_x^1$ $2p_y^1$ $2p_z^1$

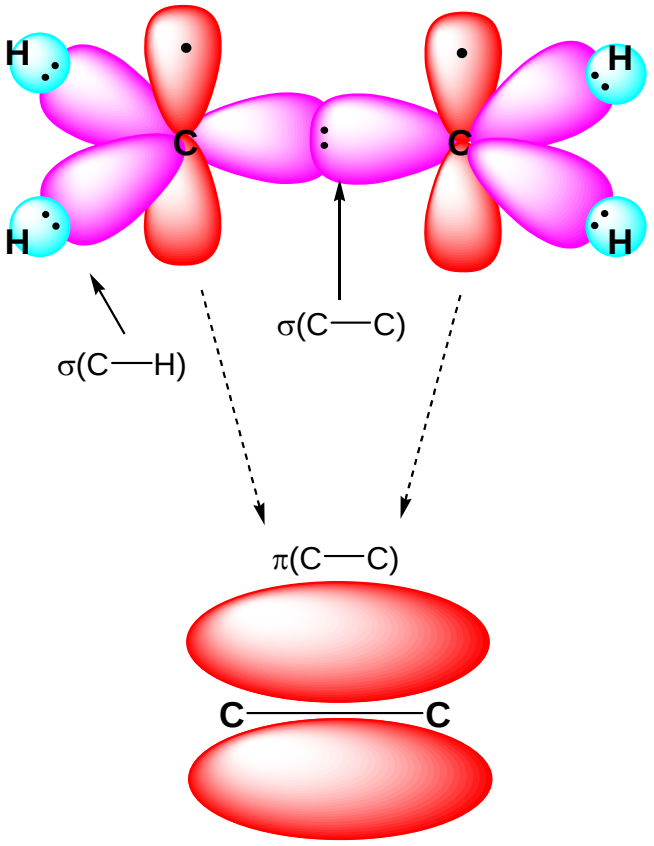




C (hybridisierter Zustand)

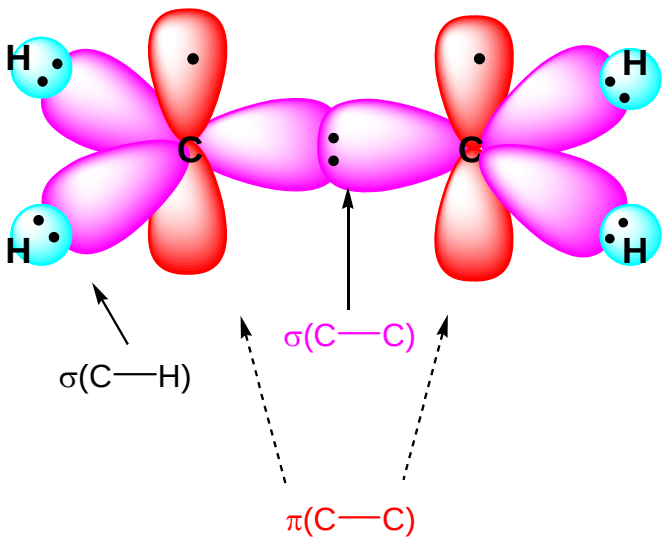


Ethen

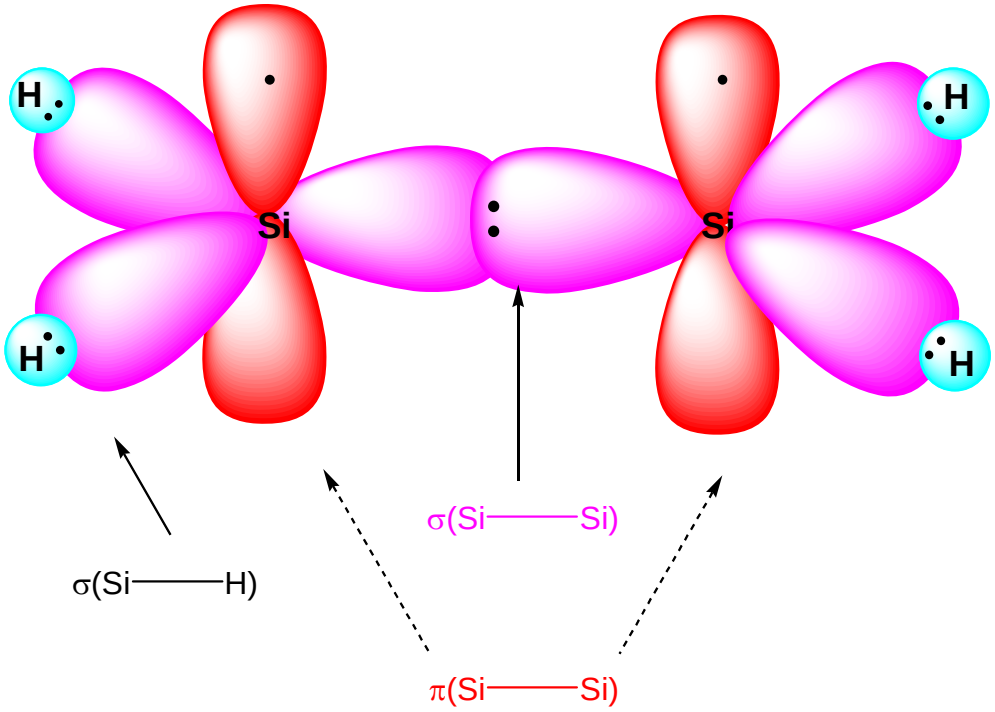


C-C-Doppelbindung

Ethen



Disilen



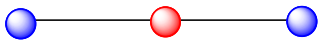
keine Wechselwirkung der p_z-Orbitale
wegen zu grossem Atomabstand
Doppelbindung wird nicht beobachtet.

"Klassische Doppelbindungsregel": Elemente der höheren Perioden können keine p_π - p_π - Doppelbindungen ausbilden.

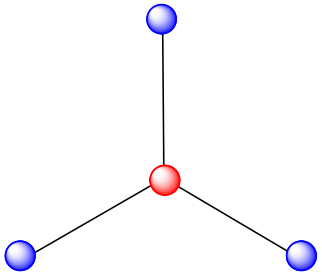
Hybridorbitale

AO	Typ	Anzahl	Räumliche Anordnung	Beispiel
s, p_x	sp	2	linear	$Be(CH_3)_2$
s, p_x, p_y	sp^2	3	trigonal-planar	BF_3
s, p_x, p_y, p_z	sp^3	4	tetraedrisch	CH_4
d_{z2}, s, p_x, p_y, p_z	dsp^3	5	trigonal-bipyramidal	PF_5
d_{z2}, d_{x2-y2}, s, p_x, p_y, p_z	d^2sp^3	6	oktaedrisch	SF_6

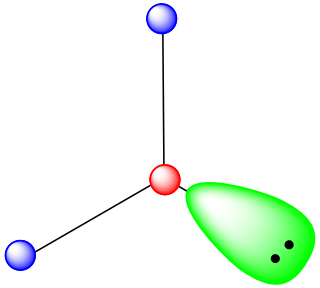
VSEPR-Modell: 2 oder 3 Aufenthaltsräume



Einsame E-Paare: 0
Molekültyp: AL_2
Geometrie: linear
Beispiele: BeH_2, CO_2, $HgCl_2$

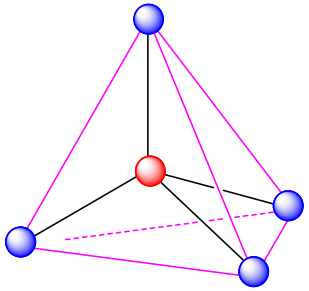


Einsame E-Paare: 0
Molekültyp: AL_3
Geometrie: trigonal-planar
Beispiele: BF_3, SO_3, NO_3^-

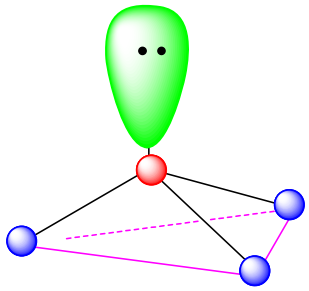


Einsame E-Paare: 1
Molekültyp: AL_2E
Geometrie: V-förmig
Beispiele: NO_2, SO_2, O_3

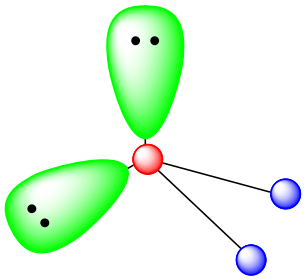
VSEPR-Modell: 4 Aufenthaltsräume



Einsame E-Paare: 0
Molekültyp: AL_4
Geometrie: tetraedrisch
Beispiele: CH_4, NH_4^+, SO_4^{2-}, $POCl_3$, SO_2Cl_2

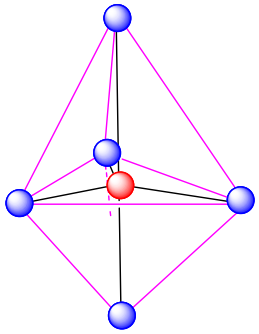


Einsame E-Paare: 1
Molekültyp: AL_3E
Geometrie: trigonal-pyramidal
Beispiele: NH_3, SO_3^{2-}, H_3O^+, $SbCl_3$

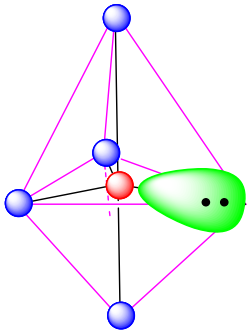


Einsame E-Paare: 2
Molekültyp: AL_2E_2
Geometrie: V-förmig
Beispiele: H_2O, H_2S, SCl_2

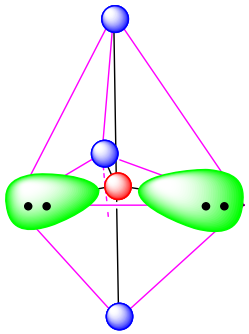
VSEPR-Modell: 5 Aufenthaltsräume



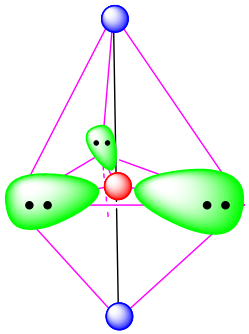
Einsame E-Paare: 0
Molekültyp: AL_5
Geometrie: trigonal-bipyramidal
Beispiele: PF_5, PCl_5, SOF_4



Einsame E-Paare: 1
Molekültyp: AL_4E
Geometrie: verzerrt tetraedrisch
Beispiele: SF_4, SeF_4, XeO_2F_2

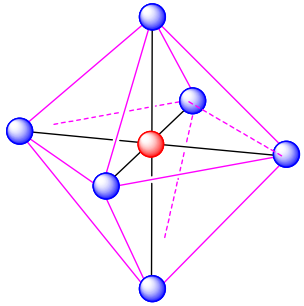


Einsame E-Paare: 2
Molekültyp: AL_3E_2
Geometrie: T-förmig
Beispiele: ClF_3, BrF_3

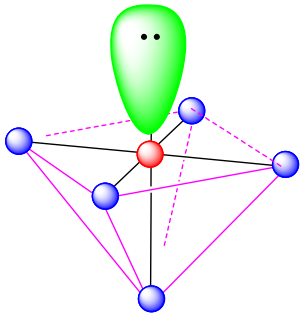


Einsame E-Paare: 3
Molekültyp: AL_2E_3
Geometrie: linear
Beispiele: XeF_2, I_3^-, ICl_2^-

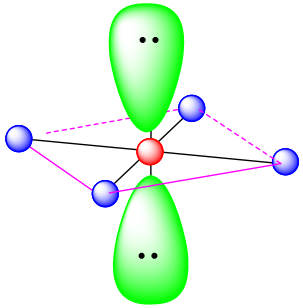
VSEPR-Modell: 6 Aufenthaltsräume



Einsame E-Paare: 0
Molekültyp: AL_6
Geometrie: oktaedrisch
Beispiele: SF_6, PCl_6^-

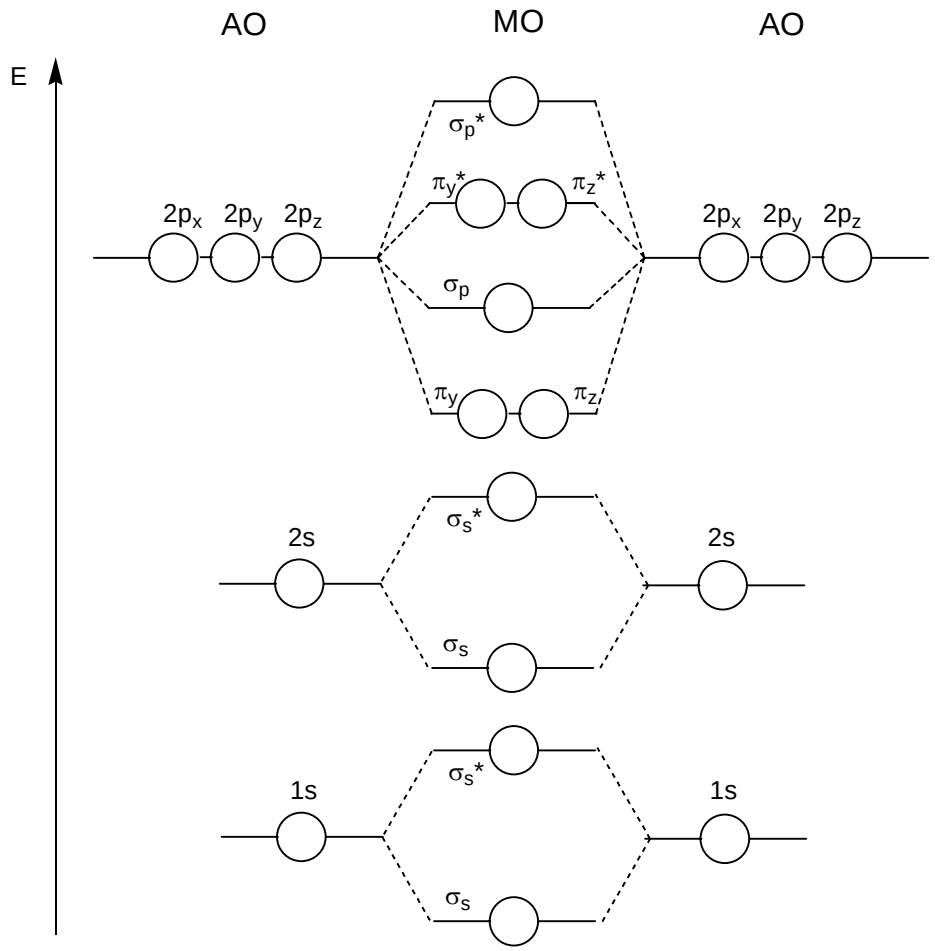


Einsame E-Paare: 1
Molekültyp: AL_5E
Geometrie: quadratisch-pyramidal
Beispiele: BrF_5, IF_5

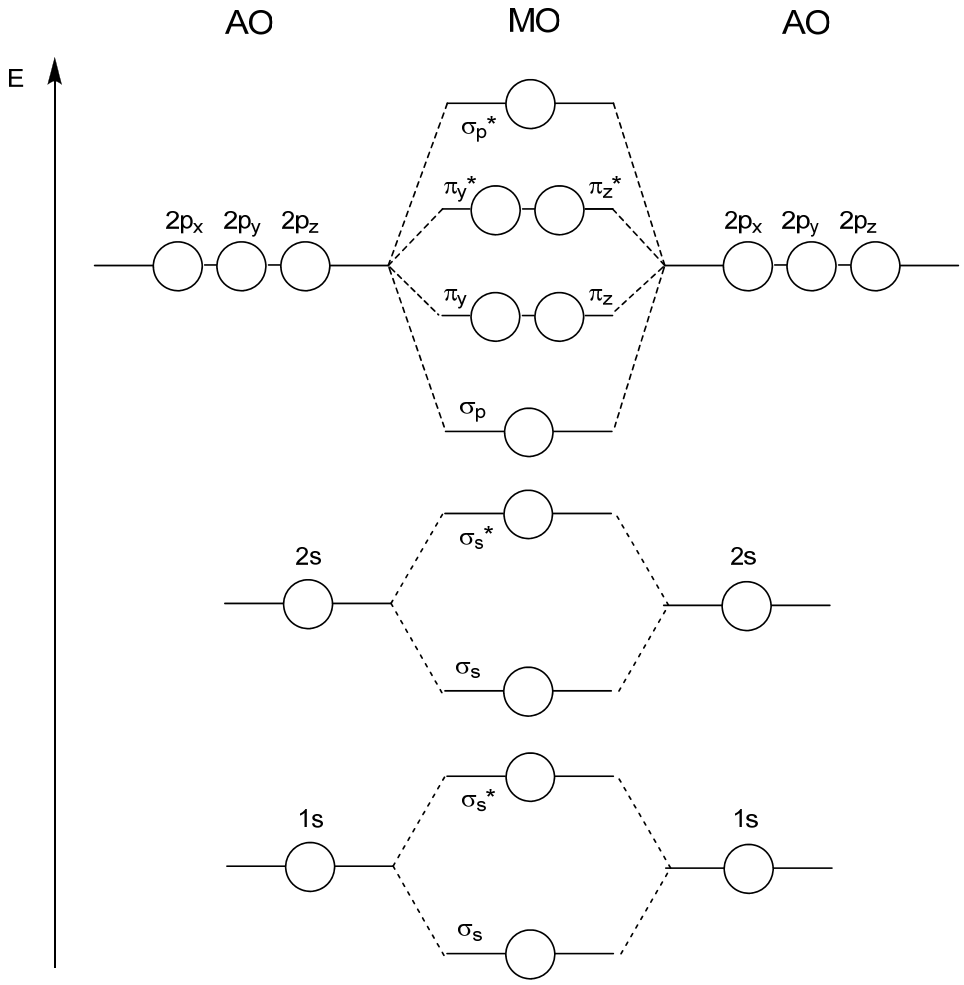


Einsame E-Paare: 2
Molekültyp: AL_4E_2
Geometrie: quadratisch-planar
Beispiele: XeF_4, ICl_4^-

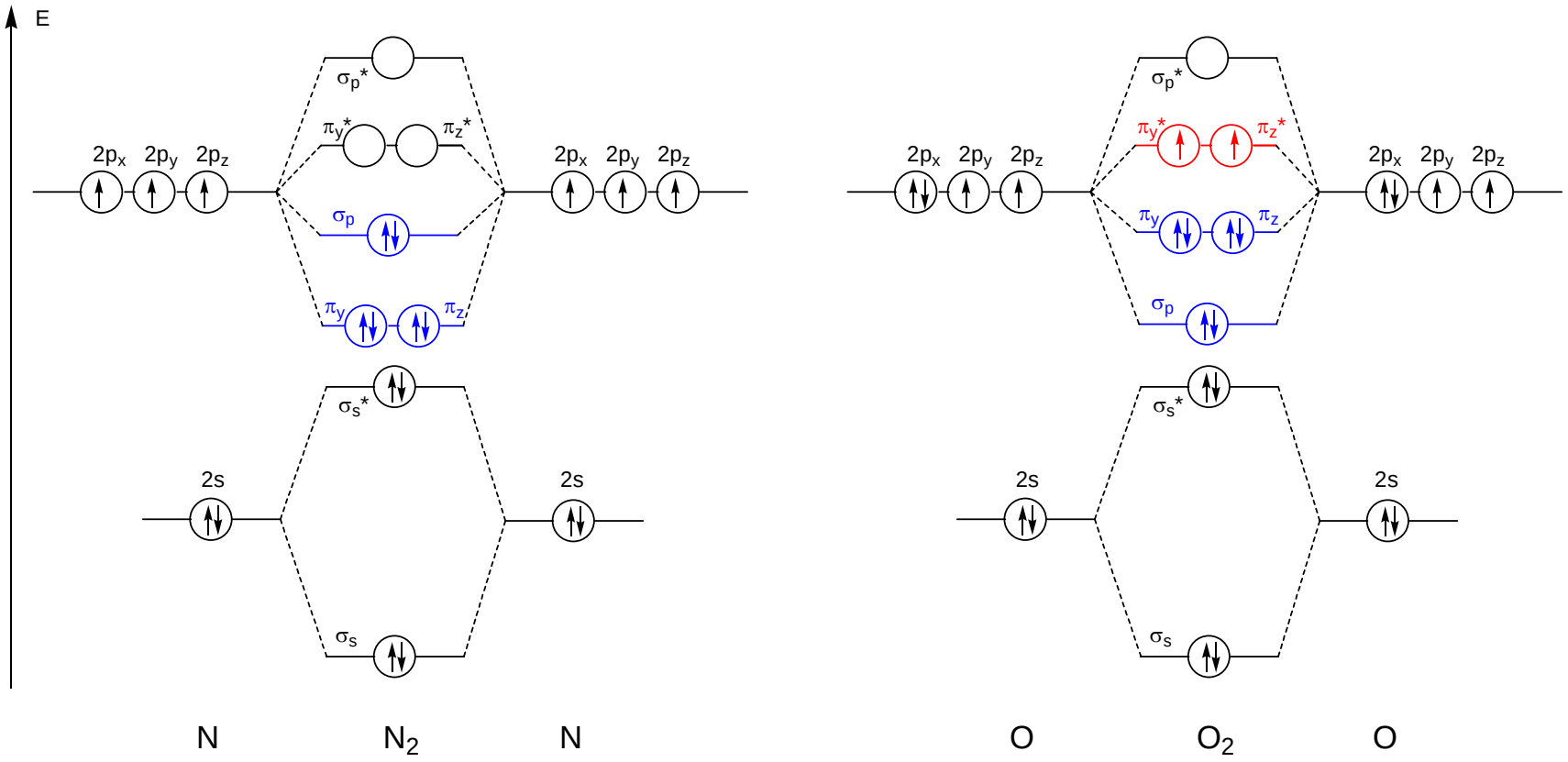
MO-Schema für zweiatomige Moleküle



MO-Schema für zweiatomige Moleküle



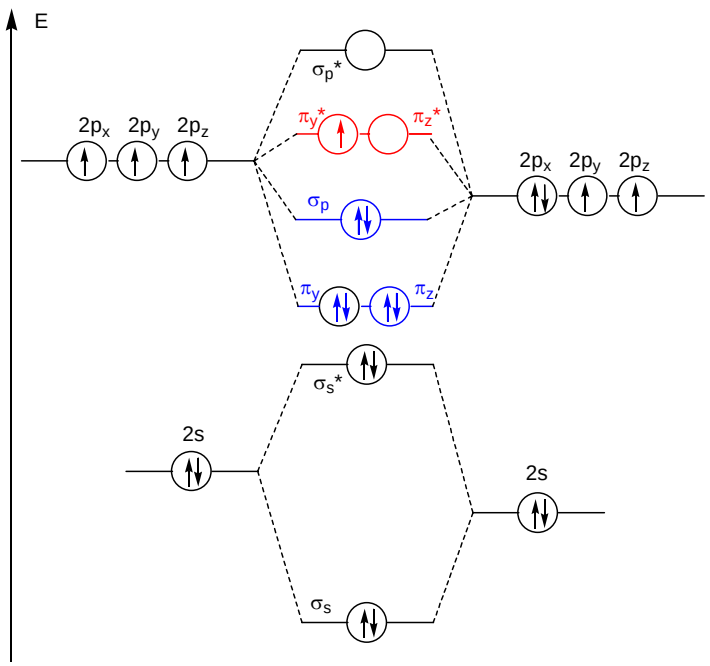
MO-Schema für zweiatomige Moleküle am Beispiel von Stickstoff und Sauerstoff

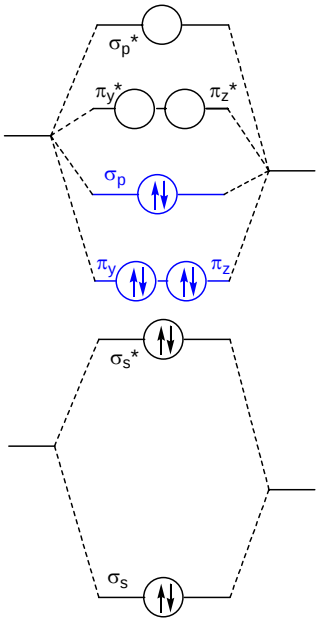


BO = 6 x 0.5 = 3

BO = 6 x 0.5 - (2 x 0.5) = 2

Vergleich der MO-Schemata von NO und NO^+





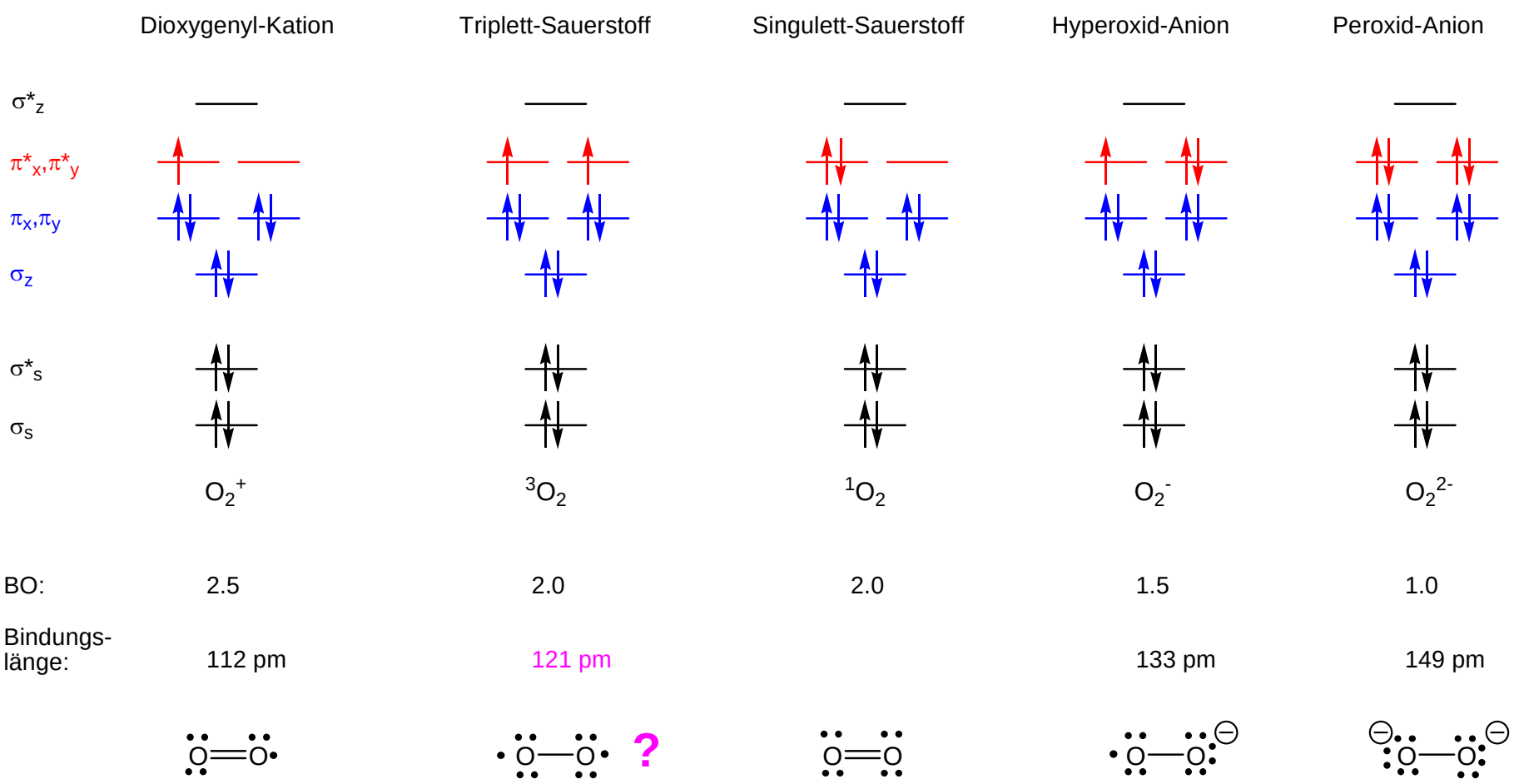
N ·N̈=Ö· O

BO = 6 x 0.5 - (1 x 0.5) = 2

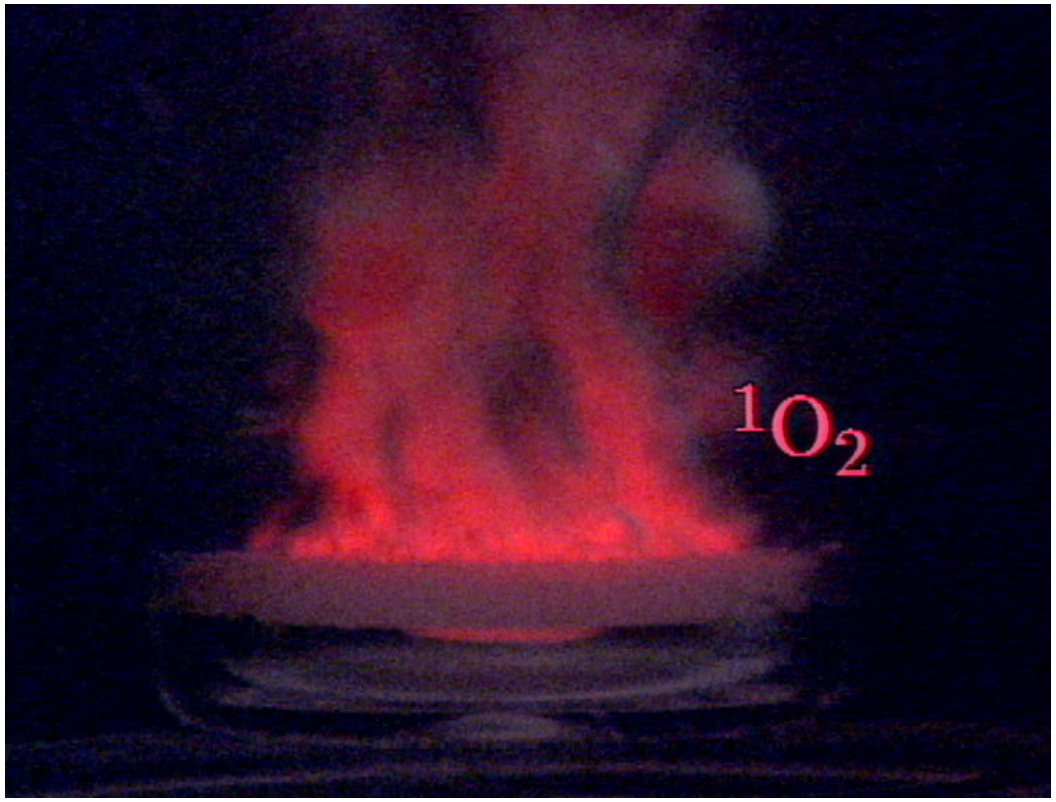
:N≡O⊕:

BO = 6 x 0.5 = 3

MO-Schemata der $O_2^{n(+)}$ - Spezies



Singulett-Sauerstoff



https://www.cci.ethz.ch/mainpic.html?picnum=-1&control=0&language=0&ismovie=1&expnum=80